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Verification of DSMC Simulations Using Spectral Analysis

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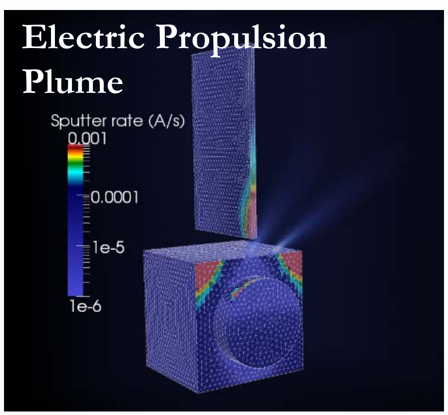
DSMC Conference, Kauai, Hawaii, USA
September 13-17, 2015

Outline

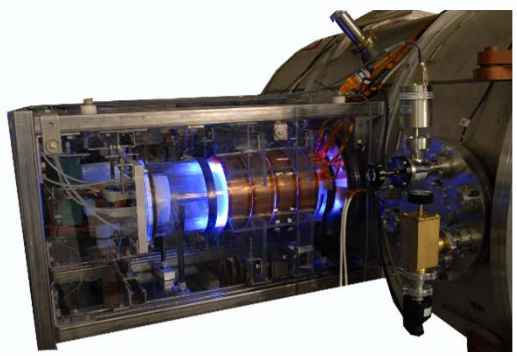
- Introduction
- Test Problem
- Chi-Square Test
- Spectral Analysis
- Conclusion / Future Work

TURF: Thermodynamics Universal Research Framework

- Unifies multiple research codes from group
  - Models of spacecraft propulsion relevant plasma at different spatial scales (1μm-100m)
    - Single fluid Magnetohydrodynamics (MHD) solver
    - Unstructured multi-fluid solver
    - Vlasov solver
    - Particle-In-Cell (PIC) with DSMC
  - Combined redundant functionality in those codes
  - Unified GPU support



Electric Propulsion Plume

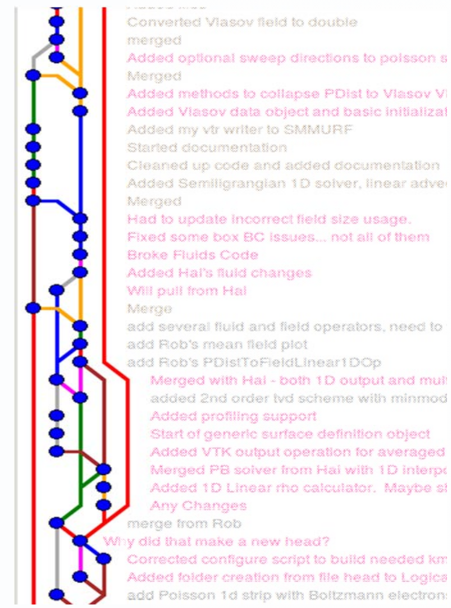

Field Reversed Configuration Plasma

Motivation / Objectives

Motivation

- Multiple developers of TURF
  - Changes to core class objects required by one model can break the others.
  - Merging different heads and making sure all the models work properly
- Automated test suites for different models

Multiple heads in Mercurial



Objectives

- Set up simple problem for testing DSMC part of TURF
- Development of efficient procedure in verifying the results

Test Problem: 1D Normal Shock

- Standalone DSMC code run on GPU
- Initial State
  - Upstream and downstream flow properties according to Rankine-Hugoniot relations
  - Discontinuous profile at t=0

$$M_2^2 = \frac{1 + \frac{\gamma - 1}{2} M_1^2}{\gamma M_1^2 - \frac{\gamma - 1}{2}},$$

$$\frac{n_2}{n_1} = \frac{u_1}{u_2} = \frac{(\gamma + 1) M_1^2}{(\gamma - 1) M_1^2 + 2},$$

$$\frac{T_2}{T_1} = 1 + \frac{2(\gamma - 1)}{(\gamma + 1)^2} \frac{\gamma M_1^2 + 1}{M_1^2} \left(M_1^2 - 1 \right)$$

	Upstream$_1$	**Downstream$_2$**
Mach Number, M	**1.20**	**0.85**
Density, n (m^{-3})	**1.00×10^{22}**	**1.30×10^{22}**
Temperature, T (K)	**293.0**	**350.1**

Test Problem: 1D Normal Shock

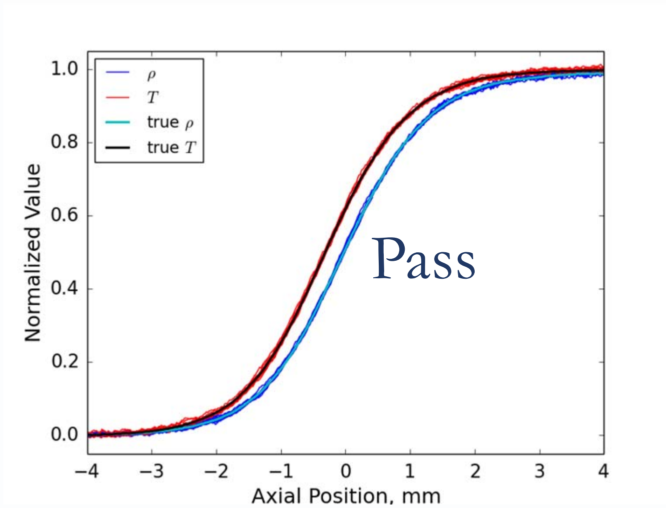
Requirements

- Fast simulation (at least < 5 hours) – less particles
- Smooth solution – more particles and time-steps

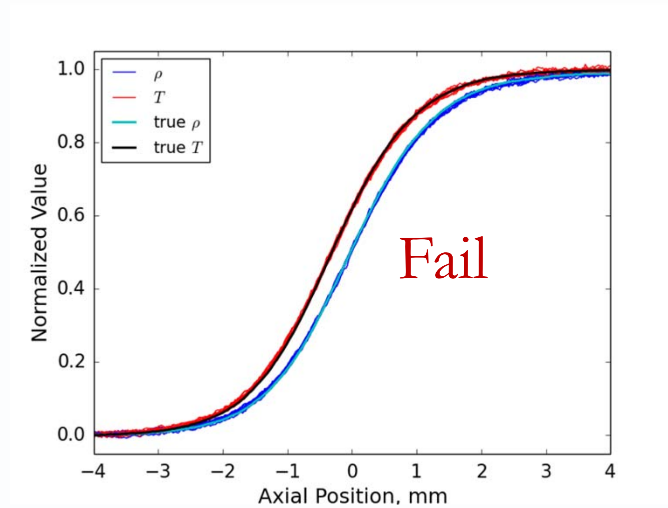
Baseline inputs: (40 mins)

- 8,000,000 Ar particles, 10,000 time-steps, 1,000 sampling cells

d_{VSS}=4.11 m^{-10}

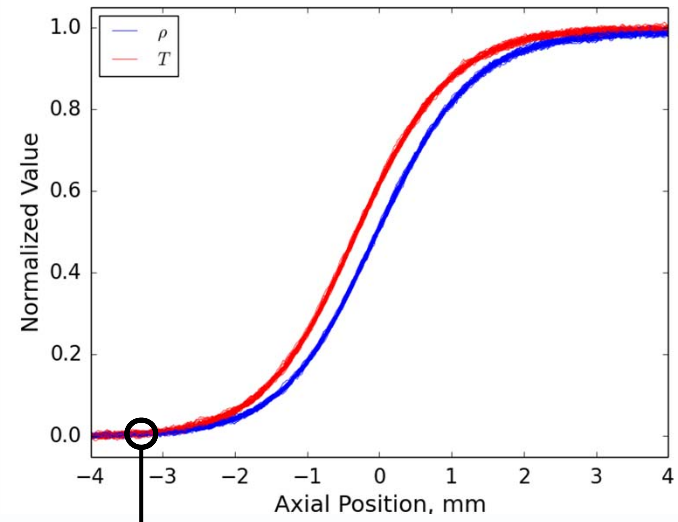


d_{VSS}=4.05 m^{-10}



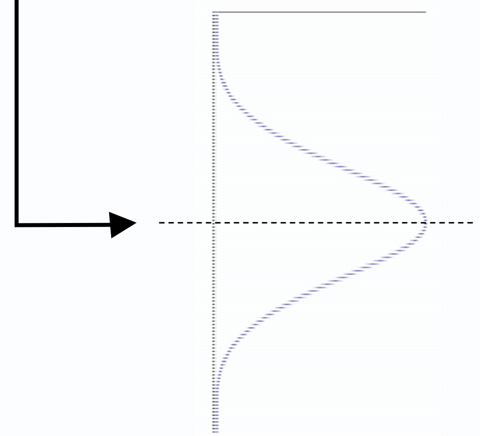
How can we systematically accept/reject results ?

1. Run the test problem M times with different random number seed



2. Deviation of results is expected to fall under normal distribution

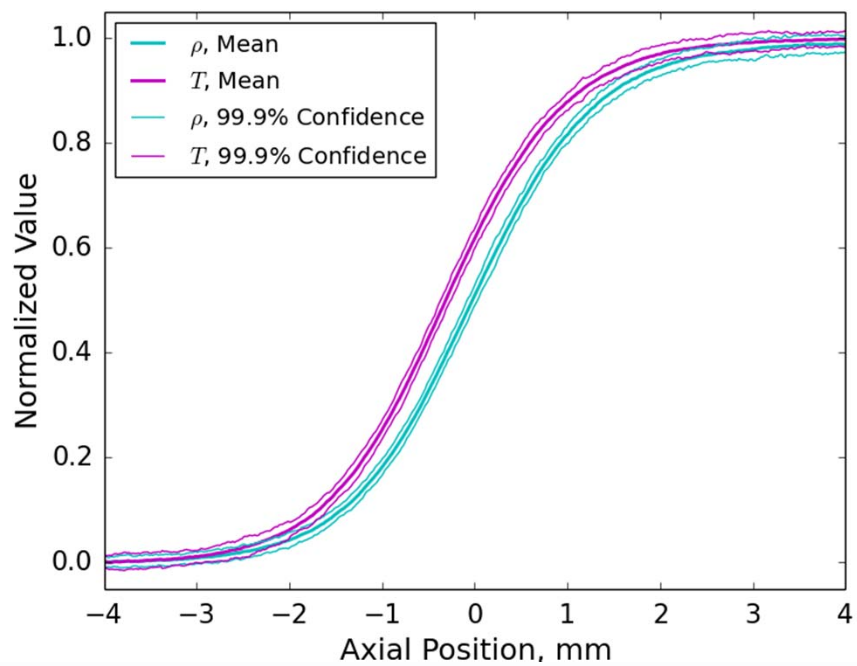
$$f(x,\mu,\sigma)=\frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



Chi-Square Test: Standard Deviation

3. Determine point-wise expected value (μ) and standard deviation (σ) for N cells

$$\mu_n = \frac{1}{M}\sum_{m=1}^{M} x_{n,m}, \quad \sigma_n = \frac{1}{M-1}\sum_{m=1}^{M}(x_{n,m} - \mu_n)^2$$



% Confidence Level	# of σs from Mean
99.9	3.2905
99	2.5758
95	1.9600
90	1.6449
80	1.2816
70	1.0364
50	0.6745

Chi-Square Test

4. For a given run, deduce a global parameter (χ) using μ and σ

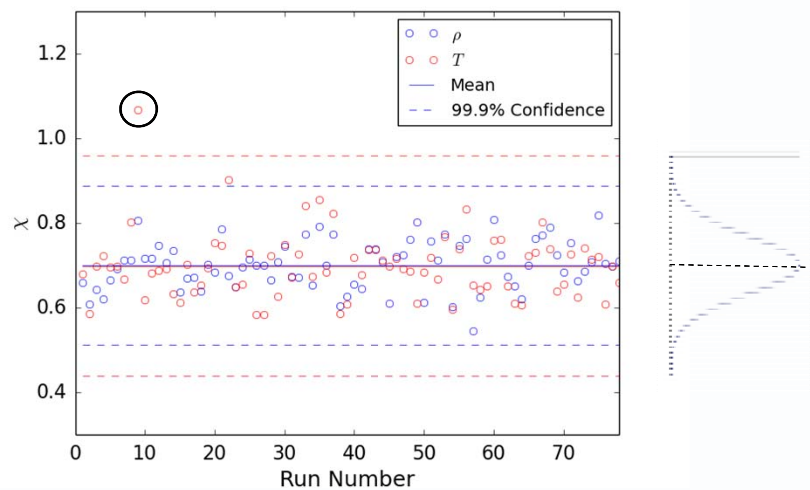
$$P = \left[\prod_{n=1}^{N} f_n \sigma_n \sqrt{2\pi}\right]^{1/N} = \prod_{n=1}^{N} \exp\left(-\frac{(x_n-\mu_n)^2}{2N\sigma_n^2}\right)$$

$$\Rightarrow -\log P = \frac{1}{2N}\sum_{n=1}^{N}\left(-\frac{(x_n-\mu_n)^2}{\sigma_n^2}\right) = \chi^2 < \chi_{\mathrm{ref}}^2$$

VSS Diameter (Angstrom)	χ	
	ϱ	T
4.11	0.753	1.02
4.00	1.10	1.06
3.90	1.33	1.31
3.80	2.79	2.64

* All runs performed with the same RNG seed

Generally increasing



Chi-Square Test: Result

- Plots of two normal distributions for different VSS diameter
  - The mean of one distribution is larger than the other with larger cross-section, but some portion of it should still overlap

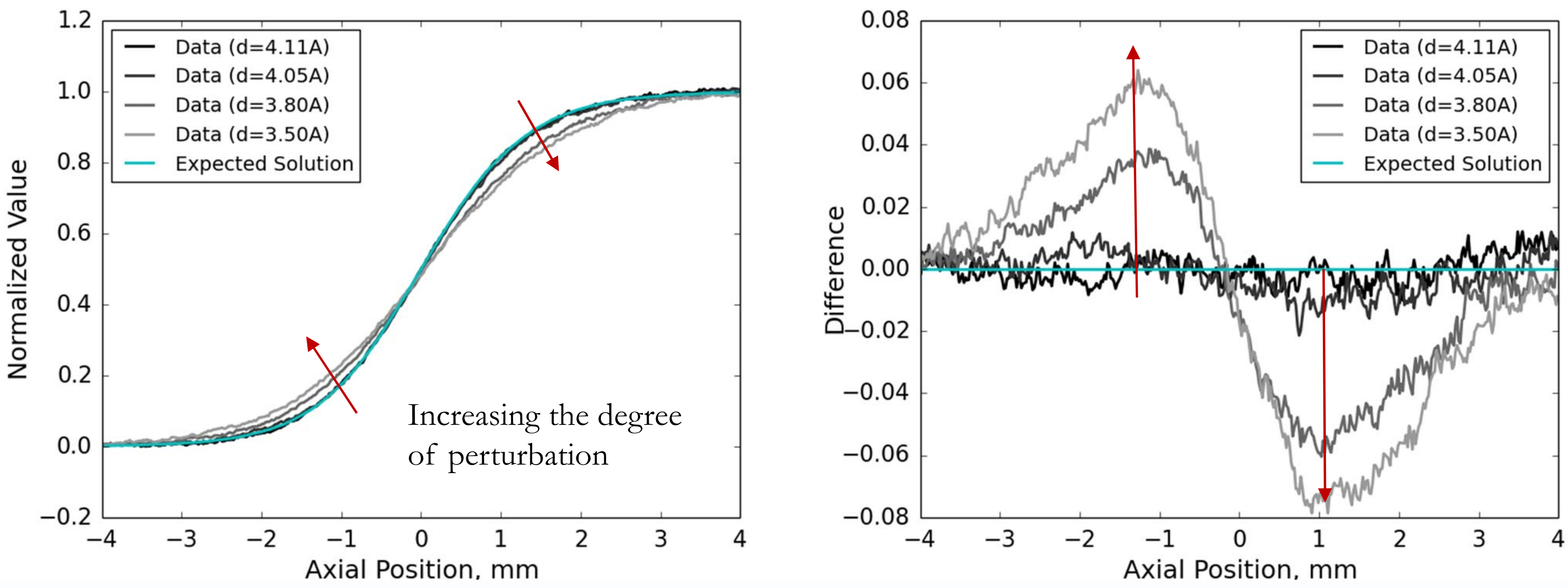
Distribution overlaps…
Could we effectively identify the distribution given a value in the overlapping region?

Remove/reduce statistical noise
- **Run more particles and time-steps?**

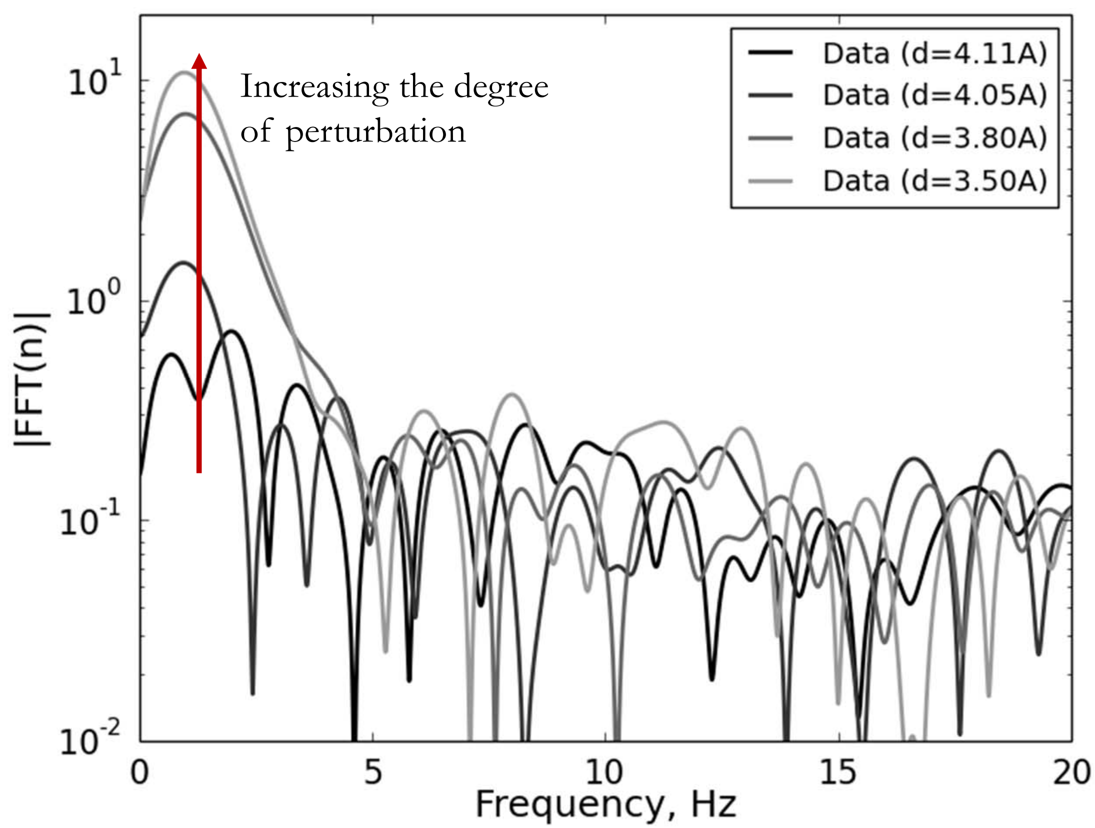
Spectral Analysis: Difference Profiles

Perform analysis in frequency space

- High frequency mode – Purely statistical
- Low frequency mode – Comes from perturbed input

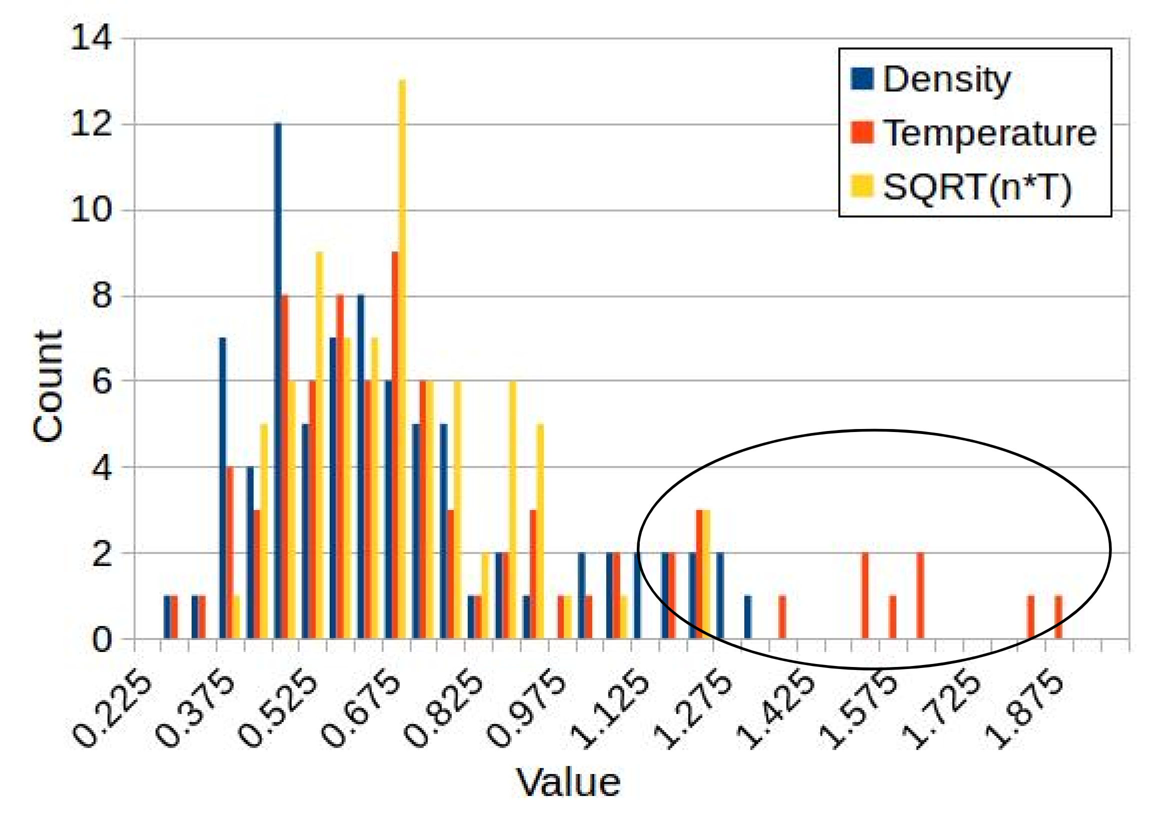


Spectral Analysis: FFT on Difference Profile



Smaller low mode amplitude as approaches the true input solution

Spectral Analysis:
Distribution of Low-Mode Amplitude



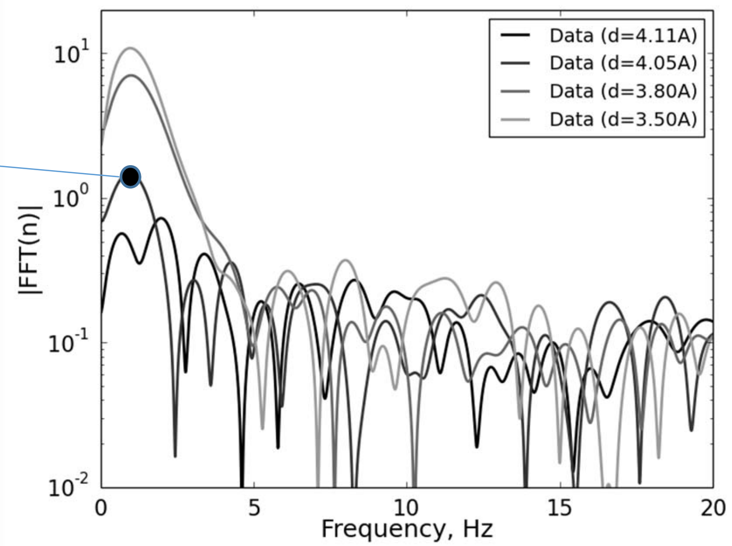
How do we deal with outliers…?

- Need to pass the runs with outliers
  - What is the probability of outliers occurring multiple times on the roll?
    - Probability of one outlier: 1%
    - Probability of outliers three times on the roll: $(1\%)^3$
- Use geometric mean to obtain the global spectral amplitude

$$\tilde{\rho} = \max|\mathrm{FFT}(\rho)|,$$

$$\tilde{T} = \max|\mathrm{FFT}(\mathrm{T})|,$$

$$\Rightarrow \max_{m=1,M} \underbrace{\left[\prod_{i=m,m+N} \sqrt{\tilde{\rho}_i \tilde{T}_i}\right]^{1/N}}_{\text{Boosting}}$$



Conclusion / Future Work

Conclusions

- Chi-Square test
  - Width of distribution is determined by the statistical noise inherent to particle simulations
- Spectral analysis
  - Strongly effective in the test problem
  - Essentially removes the effect of statistical noise in the test

Future Work

- Use the methodology in other DSMC problems to study the strength/weakness of the procedure
- Apply the knowledge in smoothing of flow properties

Thank you

Spectral Analysis

1. Perturbing the VSS diameter narrows/widens the shock width
2. Difference profile contains
    1. Low frequency mode from wrong input
    2. High frequency mode from statistical noise
3. Perform Fast Fourier Transformation (FFT) on difference profile
4. Observe the amplitude of low modes
5. Perform boosting